Manifestation of marginal Fermi liquid and phonon excitations in photoemision experiments of cuprate superconductors

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Recent ARPES experiments in cuprates superconductors show a kink in the electron dispersion near the Fermi energy. This kink coexists with a linear frequency dependence of the imaginary part of the electron self-energy. In this paper we show that both features could be accounted for if an electron-phonon interaction is included in a model where the electrons are described by a marginal Fermi liquid theory. Phonons provide the energy scale seen in the experiments but the quasiparticle weight at the Fermi level is zero. At high binding energy, in agreement with the experiment, the electron dispersion does not go to the one-electron band. We analyze the compatibility between the electron scattering rate extracted from ARPES experiment and the one extracted from transport properties. We conclude that the electron-phonon interaction relevant for transport properties is strongly screened respect to the one extracted from ARPES. This is in agreement with recent studies in the context of $1/N$ expansion on t-J model.

Recently, the improvement of momentum resolution in ARPES has generated new discussions about the interpretation of the electronic dynamic and its relation with the phenomena of high-Tc superconductivity.

In one of these experiments [1] the energy distribution curves (EDC) and momentum distribution curves (MDC) in Bi2212 (optimally doped) gave important information about the electron self-energy $\Sigma(\vec{k},\omega)$. The main result of [1] was related with the suitable linear frequency dependence of the $-Im(\Sigma(\vec{k},\omega))$ with no saturation up to frequencies of the order of $150meV$. Surprisingly, this result is very similar to the one already predicted in the early days of the HTC superconductivity [2]. In particular, Anderson [3] and Abrahams and Varma [4] related these new results with their original ideas of spin-charge separation and marginal Fermi liquid (MFL) theory respectively.

However, the subsequent ARPES experiments in Bi2212 [5,6] showed a new picture. Both papers found the presence of a kink in the electron dispersion near the Fermi surface (FS). This kink is basically a change in the slope of the dispersion, near the FS, by a factor of two and is related with an energy scale of the order of $50meV$. It is interesting to note that this low energy scale was not discussed in [1] but a close inspection of this paper shows that the kink was also observed there (see Fig.1 of [1])

A straightforward interpretation for the break in the electron dispersion is associated with a change in the Fermi velocities (FV), near the FS, by a factor of two. This can be related with a quasiparticle weight $z = 1/(1 + \lambda) \sim 0.5$, giving a characteristic coupling $\lambda \sim 1$. But if z is finite, the system behaves like a Fermi liquid (FL). On the other hand, as we mentioned above, the experiment shows that $-Im(\Sigma(\vec{k},\omega))$ is linear in ω im-

plying a zero quasiparticle weight at the FS which is not consistent with a FL picture. Therefore, it is important to investigate whether the kink is consistent only with a FL picture or it can also be interpreted in terms of non Fermi liquid theories.

The presence of this kink, which nowadays is well accepted, opens several and relevant questions: which mechanism provides the energy scale of the kink?; is $-Im(\Sigma(\vec{k},\omega))$ really linear in ω for all ω or, it deviates near the FS?; if so, is spin-charge separation or MFL the right scenario to account for this low energy breakdown of the linear behavior?.

Further experiments [7] showed the kink also in monolayer compounds LSCO and Bi2201 for several dopings (underdoped, optimally doped and overdoped). It was also shown in [5,8] that the kink and the self energy effects are rather isotropic through the Brillouin zone (BZ) and it exists below and above T_c. Another interesting feature of the kink is its evolution with temperature T. When T increases the change of the slope of the dispersion decreases, making the kink less evident.

There are two main explanations for the kink. The first one relates the kink with a magnetic excitation [9] which appears as a resonant peak in neutron scattering measurements [10] and the second one associates the kink with the electron-phonon interaction(EPHI) [11,12]. In Ref. [11] using a large-N expansion on the t-J model, it was shown that phonons are better candidates than the resonant peak to explain the low energy features associated with the kink. Besides, from the experimental point of view, as it was mentioned above, the kink is observed in optimally and overdoped regime above Tc and also in monolayer compounds. As the resonant peak was only observed in the superconducting phase of the bilayer compounds, it is problematic to associate the kink with

this magnetic resonance. Therefore, in the present paper we will take the EPHI [11,12] as the origin of the kink.

At this point we note that an EPHI can not explain the linear behavior of $-Im(\Sigma)$, measured in ARPES, with no saturation up to frequencies much larger than the Debye frequency. Recently this linear behavior in $-Im(\Sigma)$ was experimentally re-investigated for several dopings from under to overdoped [13].

One important characteristic of the electron dispersion is that, in contrast to usual metals [14,15], does not go to the one-electron band predicted from LDA calculation up to the measured energy of $200meV$ (much larger than the Debye energy). This was remarked only in [5] (to our knowledge). It will be a very important point in the present paper. Moreover, we consider that this is a clear manifestation of the existence of large $-Im(\Sigma)$ at large ω, as observed in Bi2212.

In this paper we will analyze the latest ARPES experiments in the context of the MFL. We will show that the MFL with an additional electron-phonon interaction can reproduce the ARPES results quite well. Our calculation will show that a slope-change in the dispersion of order two is also compatible with a theory that predicts a zero quasiparticle weight z at the FE. We point out that our analysis will be based manly on phenomenological grounds. It means that we will not solve or treat rigorously any microscopic Hamiltonian.

We will consider the following total self-energy $\Sigma(\vec{k},\omega) = \Sigma_{MFL}(\vec{k},\omega) + \Sigma_{e-ph}(\vec{k},\omega)$ with $\Sigma_{MFL}(\vec{k},\omega)$ the MFL self energy [2] given by $\Sigma_{MFL}(\vec{k},\omega) = \lambda[\omega log(\frac{x}{\omega_c} - i\frac{\pi}{2}x)]$. $x = max(|\omega|,T)$ and λ is a coupling constant (as we are interested in the general behavior we neglect, as a first approximation, possible vertex corrections). An important characteristic of the MFL theory is the isotropic nature of the self-energy. Σ_{e-ph} is the contribution to the self energy by the EPHI. The result for Σ_{e-ph} is not sensitive weather we use in its calculation the MFL Green function ($G_{MFL} = 1/(i\omega_n - (\epsilon(k) - \Sigma_{MFL}))$) or the simple bare electron Green function. This result is more evident when the cutoff ω_c increases. According to this remark, in the following we will present results for Σ_{e-ph} using the bare Green function.

In the following we will consider a Holstein model, with Debye frequency ω_D, for phonons and a $\vec{k}$-independent electron-phonon coupling λ^{ph}. We will also calculate Σ_{e-ph} assuming a constant electronic density of state (DOS). A more accurate calculation, which include a more realistic model for the electrons and phonons, will not change the main conclusion of the present paper.

We also need the one-electron band $\epsilon(\vec{k})$. For $\epsilon(\vec{k})$ we assume $\epsilon(\vec{k}) = -2t(cos(k_x)+cos(k_y))+4t'cos(k_x)cos(k_y)$ with $t = 150meV$ and $t'/t = 0.25$. With these parameters $\epsilon(\vec{k})$ reproduces the FS of Bi2212 [16]. The small value of these hopping parameters means that they are renormalized by electronic correlations [17,11]. We will

present calculations for doping $\delta = 0.20$ away from half-filling.

In Fig.1 we show the imaginary part of the total electron self-energy for the parameters $\lambda^{ph} = 0.75$, $\omega_D = 34.5meV$, $\omega_c = 1.8eV$ and $\lambda = (2/\pi)0.55$. We choose the parameters in order to reproduce the experimental results of [1]. Moreover, we fix the parameters in order to reproduce the difference, at zero frequency between $-Im(\Sigma)$ at $300K$ and $90K$. Using this criteria we avoid the uncertainty due to the contribution of the impurities in the samples.

The agreement between the results of Fig. 1 and the experiments is quite good with characteristic phonon parameters consistent with those previously proposed [11,19]. On the other hand we can see in Fig. 1 the overlap between the results for $T = 300K$ and $90K$ for frequencies larger than $60meV$. This fact was experimentally observed and put strong constraints on the values of the λ^{ph} and ω_D. Smaller values of these two parameters will not reproduce the mentioned overlap. In the inset of the figure we show the behavior of $-Im(\Sigma_{MFL})$ for a pure marginal Fermi liquid model at the same two temperatures. We can see the qualitatively similar behavior in ω between the inset and the main figure. Therefore as was discussed in Ref. [1], it is possible to describe the experimental result with a pure MFL model by increasing λ from our value of $\lambda = (2/\pi)0.55$ [1]. We conclude that is not possible to distinguish between the two models by solely fitting $-Im(\Sigma)$. We need, in addition the $Re(\Sigma)$. This information enters directly in the kink or break of the dispersion near the FS as we will show later. Nevertheless, if it were possible to measure $-Im(\Sigma)$ for larger energies than the ones currently available, our model predicts a splitting between the results for $-Im(\Sigma)$ corresponding to this two temperatures for $\omega >> \omega_D$. This should be a possible experimental check of the present model.

In Fig.2 we present results for the electron dispersion near the FS in the nodal direction. This dispersion was obtained as the energy position of the main peak, for a given $\vec{k}$, of the spectral function calculated with the self energy correction previously discussed. In Fig. 2 the kink is clearly observed (diamonds) at 50K near the FS. For large binding energy the electron dispersion (diamonds) does not go to the one-electron band (circles). It is also clear that, when the temperature increases from 50K to 130K, the kink is less evident like in the experiment. At larger energies than the Debye frequencies, the band goes to the pure MFL results. The figure also shows, at small temperatures, a change in the slope of the dispersion consistent with the experiment. This also means that our phonon parameters have the correct order of magnitude. The inset of the figure shows the electron dispersion corresponding to MFL at two different temperatures. From this inset we conclude that the pure MFL theory cannot reproduce the kink. There is only a small deviation (if

the temperature is large) near the FS but in the opposite direction to the experiment.

From the results shown in Fig. 2 we conclude that: to explain the kink in the context of MFL we really need an EPHI which provides an energy scale of the order of $50meV$. The presence of an EPHI to explain the kink does not mean a weakness of the MFL, on the contrary, we think that the MFL is an excellent phenomenological insight to discuss the physics of high-T_c cuprates.

In Fig. 3a we plot the inverse of the quasiparticle weight $Z = 1 - (Re(\Sigma(\omega)) - Re(\Sigma(0)))/\omega$ ($Z = z^{-1}$) for the case of only MFL Z_{MFL} (dashed line), only phonons Z_{ph} (dot-dashed line) and the total case Z (solid line). As it is well know, the quasiparticle weight goes to zero logarithmically at zero ω for the pure MFL. The solid line shows that Z goes to infinity (the quasiparticle weight goes to zero) logarithmically but also shows the structure at $\omega = \omega_D$ which is the responsible for the kink. From Fig. 3a, we can say that a change in the slope by a factor of two does not means that we really have a FL picture. In our case we can reproduce the main features of ARPES together with a zero quasiparticle weight at the FS.

One relevant question for high-Tc cuprates is weather the relaxation time $1/\tau$ measured in ARPES determines the transport properties. The DC resistivity can be calculated as $\rho = 4\pi/\Omega_p^2 \tau_{tr}$ where, in usual metals at high temperature, $1/\tau_{tr} = 2\pi\lambda_{tr}^{ph}T$ [14,18]. On the other hand, in most metals [20] the electron-phonon coupling constant λ^{ph} is nearly the same that λ_{tr}^{ph} and then, the relaxation time measured in ARPES is the same that enters in transport. The width of the Drude peak in the optical conductivity determines the quasi-particle life-time called $1/\tau^*$. For the case of EPHI in usual metals $1/\tau_{ph}^* = 2\pi\lambda_{tr}^{ph}/(1 + \lambda^{ph})T$. The experiment in cuprates [21] shows that $1/\tau^* = 1.5T$. Our previous results show that an electron-phonon coupling λ^{ph} of order 0.75 is needed in order to reproduce ARPES. If we consider, as in usual metals, that for HTC cuprates $\lambda^{ph} = \lambda_{tr}^{ph}$, we found for $1/\tau^* = 2.7T$. Then, taking into account only the electron-phonon contribution we found twice the slope of the experimental result. We have in addition a contribution to $1/\tau^*$ from the MFL which, will increase even more the discrepancies with the experiment.

Then, to explain optical data we need $\lambda_{tr}^{ph} << \lambda^{ph}$. Phonons are expected to be isotropic on the BZ and this is the reason because in usual metals $\lambda^{ph} = \lambda_{tr}^{ph}$. In their original paper Zeyher and Kulić [22] have shown $\lambda_{tr}^{ph} << \lambda^{ph}$ when the electrons are strongly correlated. The electron correlations are the responsible for vertex corrections of the EPHI. This vertex correction produces a $\vec{k}$-dependence in the final electron-phonon coupling (which was originally isotropic). As a final result, vertex corrections favor forward scattering which leads to a λ_{tr}^{ph} much smaller than λ^{ph}. In Ref. [23] it was shown

that λ_{tr}^{ph} renormalizes to around $\lambda/3$. Using a value of $\lambda_{tr}^{ph} = 0.3$ and $\lambda^{ph} = 0.75$ we obtain $1/\tau_{ph}^* = 1.07T$. We have an additional contribution from the MFL, which for our set of parameters gives $1/\tau_{MFL}^* = 1.09T$. Then, the addition of both contributions $(1/\tau_{ph}^* + 1/\tau_{MFL}^*)$ give a value in good agreement with the experiments.

There are two contributions to the resistivity, $\rho = (8\pi/\Omega_P^2)(\lambda_{tr}^{ph} + \lambda_{tr}^{MFL})T$. According to our previous discussions we will take for the transport electron-phonon coupling $\lambda_{tr}^{ph} = 0.3$. Assuming the isotropic nature of the MFL we have $\lambda_{tr}^{MFL} = 0.55$. With these two parameters and the experimental value $\Omega_p = 3eV$ we show (with circles) the temperature dependence of the DC resistivity in Fig 3b.

Our calculation compares well with overdoped samples (see figure 4 of [13] for Bi2212). It is evident from this experimental data that the resistivity is not linear in T at less for low temperatures, near Tc. It has a weak low temperature curvature similar to our results (circles) of Fig. 3b. The weakly changes between the slopes at low T given by the MFL and the slope at large T, is an additional manifestation of the small electron-phonon contribution to the transport properties.

It is very important to note that the same sample, used in the measurement for the resistivity in Fig. 4 of [13] , shows a linear behavior in ω for the $Im(\Sigma)$ and it also shows the kink in the dispersion. It will be very interesting to have experimental determinations of the resistivity at lower temperatures, for such a sample. According to our interpretation the experiment should show a linear T dependence of the resistivity due to the MFL contribution at low temperature.

The experimental data for the resistivity as a function of T for optimally doped samples both in $Bi2212$ and $YBaCuO$ does not show any curvature [24]. The behavior is surprisingly linear in T with practically no finite intercept at zero temperature. We are forced to point out that the kink also appears in these samples. Then, the question is: is λ_{tr}^{ph} exactly zero in optimally doped?.

A final discussion on this last point is in order. $1/N$ expansion on the t-J model have shown an instability toward a flux phase at a critical doping δ_c (for a given relation J/t) [25]. In [25] δ_c was identified with the optimally doped point of the phase diagram of HTC cuprates. In addition, in [22] it was shown that the electron-phonon coupling becomes more and more sharp at $\vec{k} = 0$, due to vertex corrections. This is the main reason for the decreasing of λ_{tr}^{ph} when we approach the flux-phase from the overdoped region [23]. If at δ_c the sharp electron-phonon vertex behaves like a delta function in $\vec{k}$, λ_{tr}^{ph} will be exactly zero. Our previous results give a phenomenological support to this speculation. More theoretical studies will be necessary to clarify this question [26].

In summary, we have presented a possible explanation of the recent ARPES experiments in cuprates su-

perconductors by including an EPHI in the context of a MFL theory. In this way, we have accounted at the same time for the linear ω-dependence of the imaginary part of the self-energy and for the break in the electron dispersion at a characteristic energy scale of 50 meV. We have confronted our model against the transport data and concluded that the EPHI which is relevant for transport is strongly screened respect to the one extracted from ARPES experiments. This condition is supported by strong coupling theories on the t-J model.

FIG. 2. Dispersion relation near the Fermi level in the nodal direction. Circles are the one-electron band, the squares give the MFL results as obtained from the peaks positions of the spectral functions. Triangles and diamonds show the effect of electron-phonon interaction on MFL at 130 and 50 K respectively. The inset corresponds to the MFL results at T=0 (solid) and T=300K (dotted).
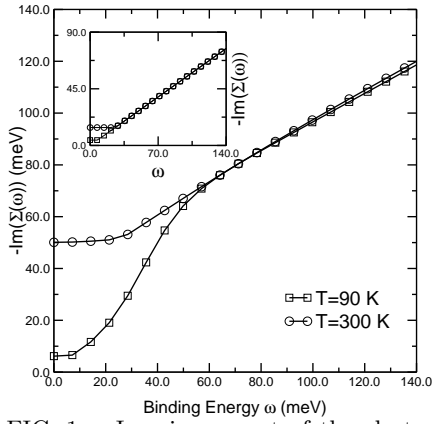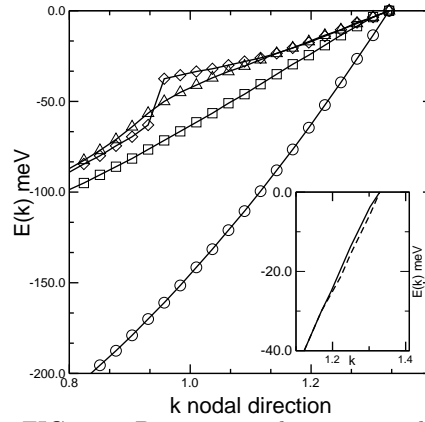

FIG. 1. Imaginary part of the electron self-energy. The inset shows the behavior of a pure MFL system where the two lines collapse in a single one at high energy. In contrast, in our model the two lines (main figure) split at frequency larger than $\sim 80 meV$ due to EPHI.
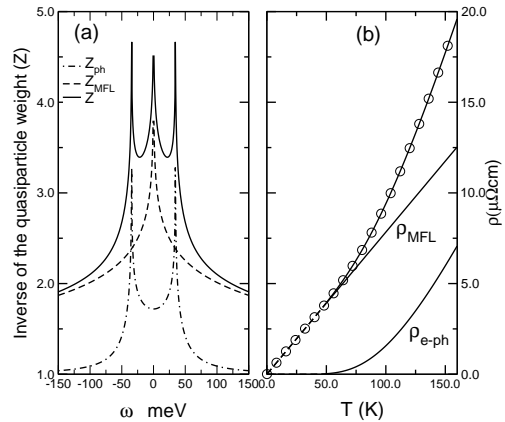

FIG. 3. (a) Different contributions to the inverse of the quasiparticle weight. (b) Temperature dependence of the electrical resistivity (circles). We show separately the contribution of the electron-phonon (ρ_{e-ph}) and MFL (ρ_{MFL}). The dotted line extrapolates the resistivity into the superconducting state.

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